

three-dimensional crystals, our results can easily be extended to the simple cubic lattice. Some of their peculiarities are caused by right angles between the interatomic bonds.

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## THE METAL-INSULATOR TRANSITION IN THE HUBBARD MODEL AT ZERO TEMPERATURE II

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We study the metal-to-insulator transition of the Hubbard model at zero temperatures in infinite dimensions. The coexistence of metallic and insulating solutions for a finite range of the interaction is established. It is shown that the metallic solution is lower in energy for any interaction in the coexistence region and that the transition is of second order.

## 1. Introduction

The correlation induced metal-insulator transition (Mott-Hubbard transition) is one of the prime examples in which strong correlations dominate the low-energy behavior of a physical system. A theoretical treatment of the problem requires an approach which is nonperturbative in the interaction. Recently, new insights into the problem were gained using the limit of infinite dimensionality.<sup>1,2</sup> It allows for a mapping of a variety of lattice models onto impurity problems in a self-consistently determined bath<sup>3,4</sup> and is, therefore, a natural way to formulate a mean-field theory of itinerant systems. While being simpler than the original problem, the resulting mean-field theory remains a formidable many-body problem which has to be solved using numerical methods. Recently the Hubbard model has been investigated by several groups using quantum Monte Carlo (QMC) simulations and self-consistent perturbation theory (PT).<sup>5,6</sup> While a combination of both methods established the existence of a Mott-Hubbard transition at a finite value of the interaction  $U$  in the paramagnetic phase of the Hubbard model at half-filling, important questions regarding the nature of the transition remain unsolved.

In a previous work,<sup>9</sup> the coexistence of metallic and insulating solutions over a finite range of values of  $U$  has been demonstrated. While the metallic solution disappears continuously at a value  $U_{c2}$ , the insulating solution disappears abruptly at a value  $U_{c1} < U_{c2}$ . At finite temperature, the difference between the free energy of the solutions is dominated by the entropy term. The large entropy, which is a

result of the degeneracy of the ground state in the insulating case, made it possible to unambiguously determine the existence of a first-order transition line close to  $U_{c1}(T)$ . As the temperature is reduced, the free energy approaches the energy, therefore an accurate evaluation of the energy is necessary. Depending on which solution is lower in energy two very different scenarios may take place: If  $E_{Ins} < E_{Met}$ , the transition will be close to  $U_{c1}$  and the sudden destruction of the metallic state implies a first-order transition even at  $T = 0$ . On the other hand, in the case  $E_{Met} < E_{Ins}$ , the metallic solution continuously merges with the insulating one at  $U_{c2}$ , and the quasiparticles display a diverging renormalized mass.<sup>9</sup>

While the limit  $T = 0$  cannot be attained by QMC simulations, within the second-order perturbative approach the energies of the two solutions are almost degenerate, making the consideration of higher-order corrections necessary. An alternative numerical approach to the problem was introduced recently: While the large  $d$  mean field equations are *functional equations* for the Green function  $G(i\omega_n)$ , an approximation can be obtained by modeling  $G(i\omega_n)$  using a finite number  $N$  of parameters, which reduces the functional equations to nonlinear algebraic equations in  $N$  unknowns. Following this idea, two different parameterizations were introduced.<sup>10,11</sup> Both take advantage of a mapping of the lattice problem onto an Anderson impurity model with a self-consistently determined bath. The  $N$  parameters that model  $G(i\omega_n)$  define the hopping amplitudes and energies of the effective electron orbitals of the bath, as will be discussed in detail in the next section. The resulting problem can then be solved at  $T = 0$  by exact diagonalization of the effective Hamiltonian. This is followed by the new determination of the set of parameters, and the procedure is iterated until convergence is attained. The method is thus nonperturbative in nature and overcomes the problems of both QMC and PT, allowing for an accurate evaluation of the energies at  $T = 0$ .

In this paper, we apply this approach to the study of the Hubbard model. We establish the coexistence of metallic and insulating solutions over a finite range of the interaction parameter  $U$  and show that at  $T = 0$  the metallic solution has lower energy than the insulating one, implying that the metal-insulator transition in the Hubbard model with semicircular density of states is of second order. This justifies *a posteriori* the relevance of the earlier studies<sup>3</sup> of this quantum critical point which captures the essence of the Brinkman-Rice transition.

## 2. Methodology

In the limit of infinite dimensionality the Hubbard model, described by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} (t_{ij} + \mu) c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right), \quad (1)$$

can be reduced to an effective impurity problem, supplemented by a self-consistency condition.<sup>4</sup> As in the previous work we focus on a Bethe lattice of infinite connectivity  $m$ , which in the noninteracting limit corresponds to a semicircular density

of states of width  $4t$ , where the hopping parameter  $t$  is rescaled in the usual way as  $t \rightarrow t/\sqrt{m}$ . Integrating out the degrees of freedom other than the origin, one obtains an effective local action of the form

$$S_{\text{eff}}[c, c^\dagger] = \sum_{\sigma} \int d\tau d\tau' c_{\sigma}^{\dagger}(\tau) G_{\sigma}^{-1}(\tau - \tau') c_{\sigma}(\tau') + U \int_0^{\beta} d\tau \left( n_{i\uparrow}(\tau) - \frac{1}{2} \right) \left( n_{i\downarrow}(\tau) - \frac{1}{2} \right). \quad (2)$$

In the following, we focus on the paramagnetic solution at half-filling ( $\mu = 0$ ). The self-consistency condition then reads  $G_{\sigma}^{-1}(i\omega_n) = i\omega_n - t^2 G(i\omega_n)$ , where  $G(i\omega_n) = - \int_0^{\beta} e^{i\omega_n \tau} \langle T_{\tau} c(\tau) c^{\dagger}(0) \rangle_{S_{\text{eff}}}$  is the local Green function of the Hubbard model once self-consistency is attained. As shown in Ref. 4 an action of the same form can be obtained from an Anderson impurity model by integrating out the conduction electrons. Note that the self-consistency condition implies that the role of the hybridization function is played by the local Green function itself. The iterative solution now proceeds as follows:  $G(i\omega_n)$  is modeled by a finite set of parameters. In terms of the impurity problem, this represents an effective bath for the impurity with a finite number of poles. This effective impurity model is then solved by exact diagonalization and a new  $G(i\omega_n)$  is calculated. A new set of parameters is then obtained from  $G(i\omega_n)$  by approximating it by a function with a number of poles equal to the number of sites in the bath (this number is, in general, smaller than the number of poles of  $G(i\omega_n)$ ). Note that this represents a further approximation of the method (beyond the effective Hamiltonian being finite). The whole process is iterated until convergence of the parameters is achieved.

Exploiting these features, two new similar algorithms were proposed recently,<sup>10,11</sup> differing basically in the way the new set of parameters is obtained, that is, how the  $G(i\omega_n)$  is parametrized by a smaller number of poles. We will consider both schemes and comment on their respective advantages and limitations.

As mentioned, the number of poles of  $G(i\omega_n)$  is in general larger than the number of sites in the bath, therefore, this approximation is an essential ingredient of the scheme. Caffarel and Krauth<sup>10</sup> proposed to obtain the new parameters by a  $\chi^2$  fit of  $G(i\omega_n)$ . Starting with an Anderson Hamiltonian of the form

$$H = \sum_{\alpha,\sigma} \epsilon_{\alpha} a_{\alpha\sigma}^{\dagger} a_{\alpha\sigma} + \sum_{\alpha,\sigma} (V_{\alpha} a_{\alpha\sigma}^{\dagger} c_{\sigma} + \text{h.c.}) + U \left( n_{c\uparrow} - \frac{1}{2} \right) \left( n_{c\downarrow} - \frac{1}{2} \right), \quad (3)$$

the self-consistency condition becomes  $l^2 G(i\omega) = \sum_{\alpha=1}^{N_{\alpha}} V_{\alpha}^2 / (i\omega_n - \epsilon_{\alpha})$ . We thus have to minimize

$$\chi^2 = \sum_{i\omega_n}^{N_{\alpha}} \left| G(i\omega_n) - \sum_{\alpha=1}^{N_{\alpha}} \frac{V_{\alpha}^2}{i\omega_n - \epsilon_{\alpha}} \right|^2, \quad (4)$$

where we sum over frequencies  $\omega_n = (2n+1)\pi T$  with small fictitious temperature ( $T = .001$ ) and large cutoff  $N_{\Omega}\Delta\omega \approx 2U$ , to obtain the new set of parameters  $V_{\alpha}$  and  $\epsilon_{\alpha}$ . Note that this Hamiltonian effectively describes an impurity surrounded by a "star" of bath electrons.

An alternative route was introduced in the context of an extended Hubbard model.<sup>11</sup> This procedure takes advantage of the fact that the Green function  $G(z)$  can be decomposed into "particle" and "hole" contributions as  $G(z) = G^>(z) + G^<(z)$  with  $G^>(z) = \langle 0|c[1/(z - (H - E_0))]c^\dagger|0\rangle$  and  $G^<(z) = \langle 0|c^\dagger[1/(z + (H - E_0))]c|0\rangle$ .

The respective contributions can be obtained from a continued fraction expansion as

$$\left\langle f_0^> / \left| \frac{1}{w \mp (H - E_0)} \right| f_0^> \right\rangle = \frac{(f_0^> / \langle f_0^> / \rangle)}{z - a_0^> / \langle - \frac{b_1^> / \langle z^2}{z - a_1^> / \langle - \frac{b_2^> / \langle z^2}{\dots}} \rangle} \quad (5)$$

where  $|f_0^>\rangle = f^\dagger|gs\rangle$ ,  $|f_0^<\rangle = f|gs\rangle$  and  $|f_{n+1}\rangle = H|f_n\rangle - a_n|f_n\rangle - b_n^>|f_{n-1}\rangle$ ,  $a_n = \langle f_n|H|f_n\rangle$ ,  $b_n^> = \langle f_n|f_n\rangle / \langle f_{n-1}|f_{n-1}\rangle$ ,  $b_0 = 0$ . This implies that  $G^>$  and  $G^<$  can be regarded as resulting from a Hamiltonian describing an impurity coupled to two chains with site energies  $a_n^> / \langle$  and hopping amplitudes  $b_n^> / \langle$ . Again the number of poles in the Green function is, in general, larger than the number of sites of the Hamiltonian and, in order to close the self-consistency, the continued fraction expansion has to be truncated. The approximation in this scheme relies on the fact that the continued fraction representation captures exactly the moments of the energy of the Hamiltonian, up to the order retained in the continued fraction. It can thus be thought of as a moment by moment fitting. This scheme has the principal advantage that it avoids the multidimensional fit of the Green function, but the disadvantage that it can be implemented practically only in the case of a semicircular density of states. In the metallic case an explicit extra site at the Fermi energy is introduced in order to better represent the low frequency region and, more importantly, to allow us to feedback a metallic bath. The hopping parameter to this extra site is calculated by a single parameter minimization of the expression

$$\chi^2(\alpha) = \sum_{i\omega_n, \alpha}^{i\omega_n, H} |G_A(i\omega_n, \alpha) - G(i\omega)|^2, \quad (6)$$

where now  $G_A(i\omega_n, \alpha) = (\alpha/i\omega_n) + (1-\alpha)G_{N_C}(i\omega_n)$ .  $G_{N_C}$  is the truncated Green function to length  $N_C = N_{\text{site}}/2$ , and  $\omega_L$  and  $\omega_H$  are low and high energy cutoffs defined by the lowest poles of  $G$  and  $G_{N_C}$ , respectively. In this case the moments will be modified by a small factor ( $\alpha$ ) which decreases as the system size is increased.

The effective Anderson model therefore reads

$$H = \sum_{\sigma} \sum_{\beta > \alpha} \left( \sum_{\alpha=1}^{N_C-1} a_{\alpha}^{\sigma} c_{\alpha\sigma}^{\dagger} c_{\beta\sigma}^{\sigma} + b_0^{\sigma} (c_{\sigma}^{\dagger} f_{\sigma} + \text{h.c.}) \right) + \sum_{\alpha=1}^{N_C-2} (b_{\alpha}^{\sigma} c_{\alpha\sigma}^{\dagger} c_{\alpha+1\sigma}^{\sigma} + \text{h.c.}) + U \left( n_{f\uparrow} - \frac{1}{2} \right) \left( n_{f\downarrow} - \frac{1}{2} \right) + \sum_{\sigma} b_0 (f_{\sigma}^{\dagger} c_{0\sigma} + \text{h.c.}) \quad (7)$$

In both schemes, ground state wave function and ground state energy of the Anderson Hamiltonian are determined by exact diagonalization (up to six sites) and the modified Lanczos technique.<sup>12</sup> Systems of up to ten sites can be handled on a workstation. The zero temperature Green function of the local site is finally obtained from a continued fraction expansion using the recursion method discussed above.

As mentioned in the introduction, a further advantage of the formulation of the problem in terms of an Anderson impurity model is the fact that the energy of the Hubbard model can be obtained directly without frequency summations using Anderson model relations. The kinetic energy per site of the Hubbard model is given as  $T = (2/\beta N) \sum_{(j,k)} \sum_{i\omega_n} t G_{jk}(i\omega_n) e^{i\omega_n 0^+}$ . Taking the limit of infinite coordination number this reduces to  $T = (2t^2/\beta) \sum_{i\omega_n} G(i\omega_n)^2 e^{i\omega_n 0^+}$ . Using the self-consistency condition as well as the fact that in the Anderson model  $(2/\beta) \sum_{i\omega_n} \sum_{\sigma} V_{\alpha}^2 / (i\omega_n - \epsilon_{\alpha}) (f_{\sigma}(i\omega_n) f_{\sigma}^{\dagger}(i\omega_n)) = \sum_{\sigma} V_{\alpha} (f_{\sigma}^{\dagger} c_{\sigma\sigma} + \text{h.c.})$ , we obtain

$$T = \sum_{\alpha\sigma} V_{\alpha} \text{Re} \langle 0 | f_{\sigma}^{\dagger} c_{\sigma\sigma} | 0 \rangle, \quad (8)$$

where  $\alpha$  labels the sites neighboring the impurity. The potential energy of the Hubbard model is obtained as

$$V = U \langle 0 | n_{f\uparrow} n_{f\downarrow} | 0 \rangle. \quad (9)$$

### 3. Results

In our analysis we have focused on two major aspects: the determination of a region where two solutions are allowed, and the resolution of controversy regarding the lowest energy solution. The two approaches considered yield a consistent picture of the transition. We are able to obtain converged metallic and insulating solutions for a finite range of the interaction  $U$  within both schemes. We further demonstrate that the metallic solution is lower in energy in the whole coexistence region. The energy difference between the solutions goes to zero as  $U_{c2}$  is approached, implying that the transition can be classified as second order. This should be contrasted with the results from second-order perturbation theory, where the two solutions

were found to cross in energy at an intermediate value of the interaction  $U$ . A point worth noticing (as was already observed within the perturbative approach) is that the energy difference between the solutions is much smaller than any energy scale of the problem. This is due to an almost perfect compensation of the gain in delocalization (kinetic) energy by the loss of energy through double occupancy (potential energy) in the metallic state compared to the insulator.

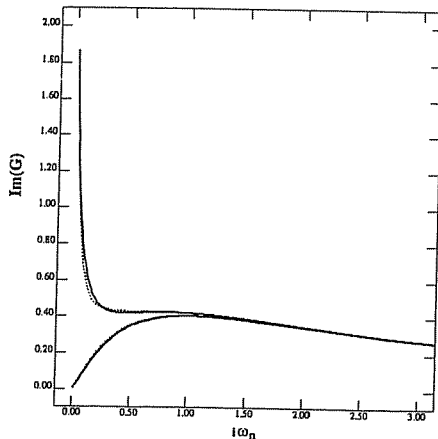


Fig. 1. Comparison of the metallic and insulating Matsubara Green functions for  $U = 2.7$ , as obtained from the two variations of the algorithm. Full line "star geometry" and dotted line "two-chain geometry" (10 sites for the metallic case and 8 sites for the insulating).

Metallic and insulating solutions for  $U = 2.7$  inside the coexistence region are, respectively, shown in Figs. 1 and 2 (the half-bandwidth  $2t$  is set equal to unity). In the first figure the Green function displays a narrow resonance at low frequency (note that the pinning condition at  $\omega = 0$  is fulfilled<sup>13</sup>), while the insulator in the second case merely consists of high energy features (upper and lower Hubbard bands). The figures also illustrate the consistency of the two schemes considered here. In both (the metallic and insulating) cases the agreement is very good. We also find that the results of both methods for the single particle Green function on the imaginary axis compare very well with the second-order perturbative calculation<sup>6</sup> and QMC<sup>6,7</sup> (the latter is discussed in Ref. 10).

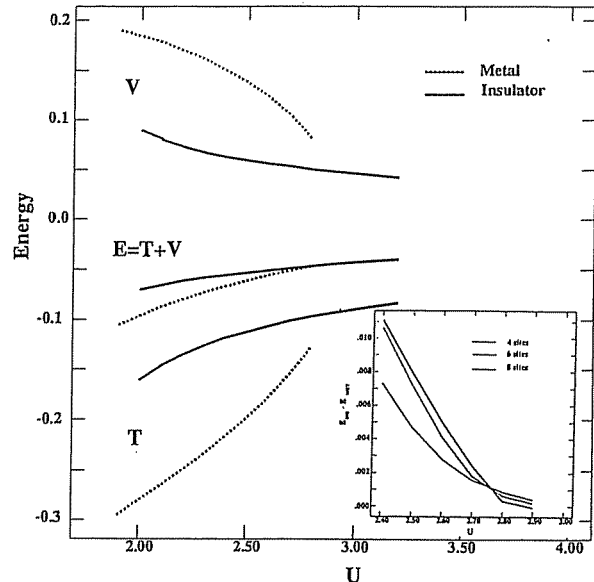


Fig. 2. Kinetic, potential, and total energy of the metallic and insulating solutions in the coexistence region. Differences between the metallic and the insulating solution are shown in the inset (from the "two-chain geometry").

The kinetic, potential and total energies for the two solutions in the coexistence region are displayed in Fig. 2. An interesting feature is the already mentioned almost perfect cancellation of delocalization and double occupancy energy. Another important observation is that while a finite size effect is apparent in the results for the kinetic and potential energy, the convergence of the total energy is much faster.<sup>14</sup> A few runs for a ten-site system show almost no difference to the results for eight sites.

The energy difference of the two solutions is shown in the inset of Fig. 2. As the critical point  $U_{c2}$  is approached from below, the finite size effects become relevant for  $U \approx 2.8$ . This limitation of the scheme is due to the fact that as the low energy

scale associated with the quasiparticle peak goes to zero close to the transition, the discrete nature of the approximation starts playing an important role and the Kondo resonance is represented by only a single pole.

The smallness of the difference in energy between the metal and the insulator can be understood from the picture of a second-order critical point where the metallic and insulating solutions merge with a vanishing scale  $\Delta \sim U_{c2} - U$ . The problem can be formulated from a variational point of view, with the free energy  $F$  becoming an extremum at the metallic and insulating solutions, i.e.  $(\delta F / \delta G_M) = (\delta F / \delta G_I) = 0$ . Since the two solutions merge at the point  $U_{c2}$ ,  $F$  can be expanded in power series of  $G_M - G_I$  as

$$F_M - F_I = \frac{\delta^2 F}{\delta G^2} (G_M - G_I)^2. \quad (10)$$

As the difference between the metallic and the insulating solution is parameterized by  $\Delta$ , and the second derivative vanishes at the critical point as  $\Delta$ , it follows that the energy difference goes to zero as  $\Delta^2$ . The critical region cannot be accessed by the present method. In order to capture the vanishing energy scale, a higher resolution (i.e. an effective bath with more sites) is needed.

Finally, we would like to comment on the disappearance of the insulating solution at  $U_{c1}$ . From the "two-chain" scheme, the insulating solution is found to persist all the way down until the gap closes. This differs from the results of the perturbation theory and resembles the Hubbard III scenario for the destruction of the insulating state.<sup>16,a</sup> In the case of the "star configuration," while a converged insulating solution can be obtained at values of the interaction  $U$  well below  $U_{c2}$ , the question of the closing of the gap cannot be answered conclusively.

#### 4. Conclusions

We have resolved the standing questions regarding the metal-to-insulator transition in the Hubbard model in infinite dimensions, using a powerful algorithm to obtain Green functions at zero temperature.<sup>b</sup> We were able to demonstrate the existence of a region in which metallic and insulating solutions coexist, which is in agreement with previous results, and showed that the metallic solution is always lower in energy. This implies that while at finite temperature the transition is first order, it becomes second order at  $T = 0$ , similar to the work of Brinkman and Rice in the context of the Gutzwiller approximation.<sup>3,15</sup> Since the method presented is very general as well as simple, especially when compared to Monte Carlo simulations, it is an appealing approach to the study of strongly correlated electron systems.

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<sup>a</sup>In a recent preprint, Gros *et al.* (SISSA # cond-mat/9312031) studied the insulating solution at zero temperature using a finite-size cluster method and obtained similar results on the issue of the disappearance of the insulator.

<sup>b</sup>Note that this can also be used to obtain the dynamical correlation functions like the spin-spin correlation function.